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INVESTIGATION OF SCALAR FILTERED DENSITY FUNCTION IN TURBULENT PARTIALLY PREMIXED FLAMES

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SUMMARY

The filtered mass density function (FMDF) of mixture fraction and other filtered variables used in large-eddy simulation of turbulent combustion are studied using measurement data obtained in turbulent partially premixed methane/air (Sandia) flames. For SGS scalar variance small compared to its mean, the FMDF is not far from Gaussian and the SGS scalar is well mixed. For large SGS variance, however, the FMDF becomes bimodal and the conditionally filtered scalar dissipation is bell-shaped, indicating the existence of a diffusion (dissipation) layer structure, which is similar to the mixture fraction profile in the counter-flow model for laminar flamelets. The conditionally filtered temperature near the stoichiometric mixture fraction decreases progressively with increasing SGS scalar variance. Furthermore, local extinction events appear to occur mostly when the SGS scalar variance is large, suggesting the possibility of flamelet extinction. The results suggest that the mixing regimes and the associated mixture fraction structure could potentially have strong influences on the combustion regime and extinction/reignition in turbulent nonpremixed flames.

TECHNICAL DISCUSSION

LES has been recognized as a very promising approach to modeling turbulent combustion. In LES the subgrid-scale (SGS) scalar mixing and the resulting instantaneous distribution of scalar values in each grid volume (i.e., the filtered density function) must be faithfully represented in order to accurately predict the chemical reaction rate. The present study investigates issues in using this approach, including SGS mixing and turbulence-chemistry interaction, which play crucial roles in LES of nonpremixed combustion.

Our previous studies of the SGS mixing of a conserved scalar in nonreacting jets (Tong 2001, Rajagopalan and Tong (2003), Wang and Tong (2002, 2004), Wang et al. 2004) have shown that the SGS scalar at a fixed location has qualitatively different FDF shapes and structures depending on the *instantaneous* SGS scalar variance. When the SGS variance is small compared to its mean value, the SGS scalar has close to Gaussian distributions, indicating well mixed SGS scalar fields. The SGS turbulence is in quasi-equilibrium, i.e., the production of the SGS variance is equal to or smaller than the SGS dissipation rate. When the SGS variance is large compared to its mean value, the conditional SGS structure on average resembles that of a counter-flow diffusion flame, which is a model for laminar flamelets. The SGS scalar has bimodal distributions, indicating highly nonpremixed SGS scalar fields. In a nonpremixed flame this would indicate that the fuel lean and rich regions of the SGS fields are highly segregated. There is a sharp interface separating the two regions, across which there is a large scalar value jump (can be as large as the integral-scale fluctuations). In addition the SGS scalar is in nonequilibrium.

The well-mixed SGS mixture fraction fields with close-to-Gaussian distributions and the highly nonpremixed SGS fields with bimodal distributions can potentially have strong influences on the flame structure. In this study we investigate the SGS mixing of the mixture

fraction in turbulent partially premixed flames and examine the effects of the different SGS mixture distributions and structures on the flame structure. We investigate the characteristics of the filtered mass density function (FMDF) of the mixture fraction

$$F_{\xi L}(\hat{\xi}; \mathbf{x}, t) = \langle \rho(\mathbf{x}, t) \delta(\xi - \hat{\xi}; \mathbf{x}, t) \rangle_{\ell} = \int \rho(\mathbf{x}', t) \delta(\xi - \hat{\xi}; \mathbf{x}', t) G(\mathbf{x} - \mathbf{x}') d\mathbf{x}', \quad (1)$$

and the mixing term in its transport equation, the conditionally filtered scalar dissipation rate,

$$\langle \chi | \xi \rangle_{\ell} = \langle D \frac{\partial \xi}{\partial x_j} \frac{\partial \xi}{\partial x_j} | \xi \rangle_{\ell}, \quad (2)$$

where ξ , ρ , and D are the mixture fraction, the fluid density and the diffusivity for the mixture fraction, respectively. The subscripts ℓ and L denote conventional and Favre filtered variables respectively. The dependences of $F_{\xi L}$ and $\langle \chi | \xi \rangle_{\ell}$ on the different mixing process will be studied. We also analyze the conditionally filtered temperature $\langle T | \xi \rangle_{\ell}$ and examine conditional SGS temperature samples to study the effects of SGS mixing on flames structure.

Experimental data and processing procedures

We use experimental data obtained in piloted turbulent partially premixed methane with a 1:3 ratio of CH_4 to air by volume (Sandia flame D and E, (Karpetis and Barlow (2004, 2004)). Their measurements employed combined line-imaging of Raman scattering, Rayleigh scattering, and laser-induced CO fluorescence. Simultaneous measurements of major species (CO_2 , O_2 , CO , N_2 , CH_4 , H_2O , and H_2), mixture fraction (obtained from all major species), temperature, and the radial component of scalar dissipation rate were made. The mixture fraction is calculated using a variation of Bilger's definition, which has been modified by excluding the oxygen terms. The length of the imaging line is 6.0 mm with a resolution of 0.2 mm.

Measurements of the filtered density functions require spatial filtering of scalar fields. In this research, both one-dimensional filtering will be employed. The filter sizes Δ employed in this work are 3.0 and 6.0 mm.

Results

The FMDF and other SGS variables are analyzed using their conditional averages. We use the Favre filtered mixture fraction,

$$\langle \xi \rangle_L = \langle \rho \xi \rangle_{\ell} / \langle \rho \rangle_{\ell}, \quad (3)$$

and the Favre SGS scalar variance,

$$\langle \xi'^2 \rangle_L \equiv \frac{1}{\langle \rho \rangle_{\ell}} \int F_{\xi L}(\hat{\xi}; \mathbf{x}, t) (\xi - \langle \xi \rangle_L)^2 d\xi = \langle \rho \xi^2 \rangle_{\ell} / \langle \rho \rangle_{\ell} - \langle \xi \rangle_L^2, \quad (4)$$

as conditioning variables. The SGS variance value normalized by its ensemble mean is denoted by $\langle \xi'^2 \rangle_L^*$.

The conditional mixture fraction FMDF for flame D for several SGS variance values is shown in Fig. 1. The results for flame E (not shown) are similar. The Favre filtered mixture fraction is set to the stoichiometric mixture fraction, $\xi_s = 0.35$, to maximize the probability of the SGS field containing reaction zones. For $\langle \xi'^2 \rangle_L^* \ll 1$ the conditional FMDF, $\langle F_{\xi L} | \langle \xi \rangle_L, \langle \xi'^2 \rangle_L^* \rangle$, is generally unimodal and probably not very far from Gaussian. This suggests that the SGS scalar is likely to follow the Kolmogorov's cascade picture. Therefore, when the filter scale decreases the SGS fluctuations become smaller, suggesting that the burden on the SGS mixing models is reduced.

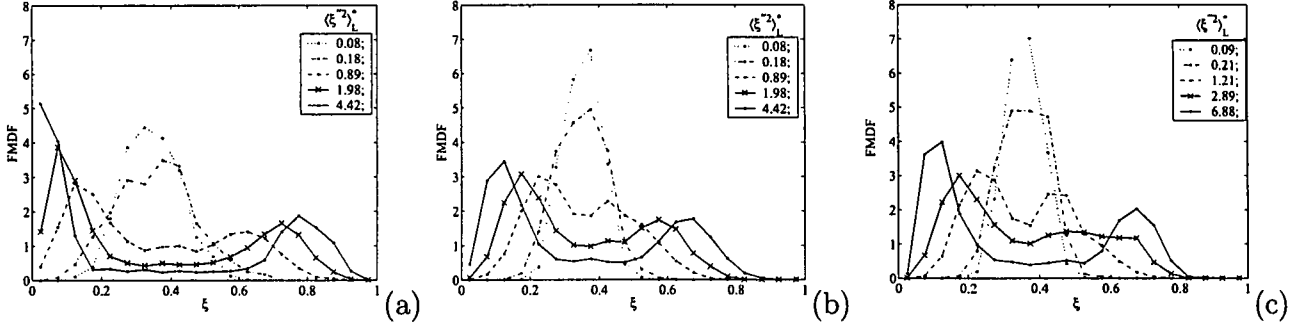


Figure 1: The mean conditional scalar FMDf for Sandia flame D for $\langle \xi \rangle_L = \xi_s$ and several $\langle \xi''^2 \rangle_L^*$ values (specified value $\times [0.67, 1.49]$). (a) $x/D=15$, $\Delta = 6.0mm$; (b) $x/D=15$, $\Delta = 3.0mm$; (c) $x/D=30$, $\Delta = 6.0mm$

For $\langle \xi''^2 \rangle_L^*$ close to or larger than one, the FMDf becomes bimodal and the bimodality is stronger for larger SGS variance. This indicates that the SGS mixture fraction is highly nonpremixed. Therefore, the rich and lean mixtures in a grid cell are essentially segregated. The bimodal FMDf is also similar to the scalar FDF for large SGS variance observed in nonreacting flows. The SGS scalar is not well described by Kolmogorov's turbulence cascade picture.

In contrast to the unimodal FMDf, the dependence of the bimodal FMDf on the filter scale is much weaker. The FMDf at $x/D = 15$ for a filter size of 3.0 mm shown in Fig. 1(b) has the same characteristics as that for a 6.0 mm filter. Therefore, large scalar value jumps exist in the SGS scalar regardless of the filter scale as long as the filter scale is larger than the scalar dissipation length scale, which is generally the case in LES. This suggests that when the SGS variance is large, the burden on the mixing model to correctly model the SGS mixing is not reduced when the filter size is decreased.

The results show that the statistical structure of the SGS mixture fraction is different for small and large SGS variance values. The difference of the ξ values between the two FMDf peaks is often larger than the equilibrium reaction zone width in the ξ space for the methane flames studied in this work ($\Delta \xi_R \approx 0.23$ (Frank et al. 2002)). Therefore, such a mixture fraction structure is likely to support laminar flamelets. This is in contrast with the well-mixed SGS mixture fraction for small SGS variance where the turbulence cascade is likely to dominate and the dissipation-scale scalar fluctuations are predicted by the Kolmogorov-Obukhov-Corrsin theory. Therefore, such a SGS mixture fraction is likely to result in distributed reaction zones.

The conditionally filtered scalar dissipation $\langle \chi | \xi \rangle_\ell$ (not shown) also has qualitatively different dependences on the mixture fraction for small and large SGS variance. For small $\langle \xi''^2 \rangle_L^*$ it depends relatively weakly on ξ , except near $\xi = 0$ and 1. This is consistent with the FMDf being unimodal and not far from Gaussian. For large $\langle \xi''^2 \rangle_L^*$, $\langle \chi | \xi \rangle_\ell$ becomes bell-shaped, with the maximum at the ξ value where the bimodal FMDf has a dip, indicating that there is an interface between the highly segregated SGS mixture fraction regions and that the interface is sharp and is essentially a diffusion layer. The FMDf and the conditionally filtered dissipation results suggest that the SGS mixture fraction structure is similar to that in the counter-flow model for laminar flamelets.

The conditionally filtered temperature $\langle \langle T | \xi \rangle_\ell | \langle \xi \rangle_L, \langle \xi''^2 \rangle_L^* \rangle$ for the Sandia flame D at $x/D = 7.5$ and 15 are shown in Fig. 2. For small SGS variance the conditionally filtered temperature is close to the equilibrium values. As the SGS variance increases, the temperature begins to decrease, especially near the stoichiometric mixture fraction. The magnitude

of the temperature reduction is considerably smaller for $x/D = 7.5$ than for $x/D = 15$ and $x/D = 30$ (not shown). Because the jump in mixture fraction is large for large SGS variance, the decreases in temperature under such conditional are likely caused by straining or extinction of laminar flamelets.

It is important to note that although the conditionally filtered temperature in Fig. 3 is somewhat similar to the conditional mean temperature obtained by using χ_s as the conditioning variables[?], conditioning on the SGS variance provides additional information than conditioning on the dissipation rate alone. This is because the SGS variance enables conditional sampling of the structure of the SGS mixture fraction, thereby allowing the effects of the mixture fraction structure on the flame structure to be studied.

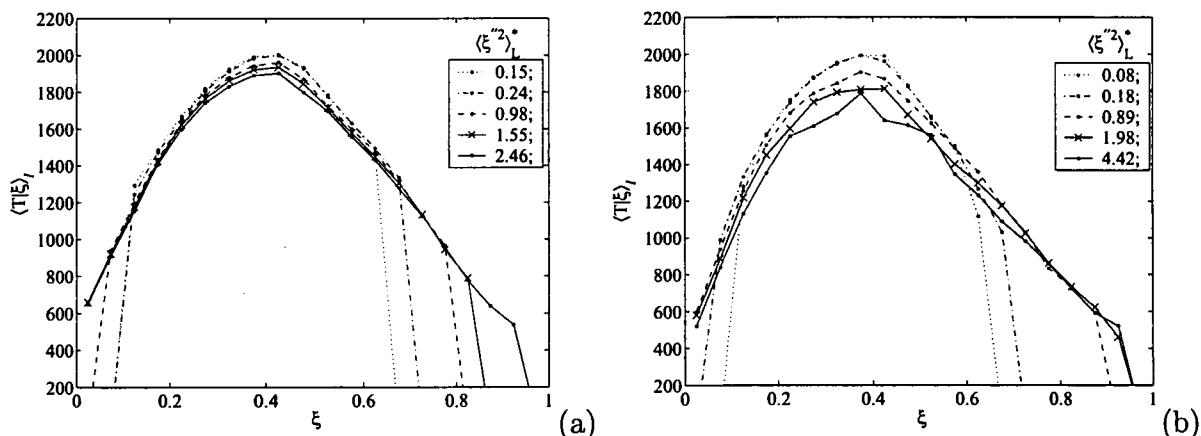


Figure 2: The mean conditionally filtered temperature for flame D for $\langle \xi \rangle_L = \xi_s$ and several $\langle \xi''^2 \rangle_L^*$ values. (a) $x/D=7.5$, $\Delta = 3.0mm$; (b) $x/D=15$, $\Delta = 6.0mm$.

REFERENCES

- Frank, J. H., Kaiser, S. A., and Long, M. B. (2002) Reaction rate, mixture fraction, and temperature imaging in turbulent methane/air jet flames, *Proc. Combust. Inst.* **29**, 2687 .
- Karpetsis, A. N. and Barlow, R. S. (2002) Measurements of scalar dissipation in turbulent piloted methane/air jet flames, *Proc. Combust. Inst.* **29**, 1929.
- Karpetsis, A. N. and Barlow, R. S. (2004) Measurements of flame orientation and scalar dissipation in turbulent partially premixed methane flames, *Proc. Combust. Inst.* **30**, 665.
- Rajagopalan, A.G. and Tong, C. (2003) Experimental investigation of scalar-scalar-dissipation filtered joint density function and its transport equation. *Phys. Fluids*, **15**, 227–244.
- Tong, C. (2001) Measurements of conserved scalar filtered density function in a turbulent jet. *Phys. Fluids* **13**, 2923–2937.
- Wang, D. and Tong, C. (2002) Conditionally filtered scalar dissipation, scalar diffusion, and velocity in a turbulent jet. *Phys. Fluids* **14**, 2170–2185.
- Wang, D. and Tong, C. (2004) Experimental investigation of velocity-scalar filtered density function for LES of turbulent combustion. *Proc. Combust. Inst.* In press.
- Wang, D., Tong, C., and Pope, S.B. (2004) Experimental investigation of velocity filtered density function for large eddy simulation. *Physics of Fluids* **16**, 3599–3613.